Muhammad Fahad **Arshad**

Postdoctoral Researcher · PhD, Engineering Thermophysics

Ben Guerir, Morocco

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"Advancing sustainable energy solutions through computational catalysis and hydrogen production research"

Summary

Computational catalysis researcher blending heterogeneous experimentation with high-performance modelling (DFT, MD, AI/ML) to design low-carbon hydrogen and CO_2 utilisation pathways. Delivered reactor innovations, cross-functional collaborations, and data-driven workflows that accelerated catalyst discovery from concept to pilot scale.

Education

New Technology Lab, University of Chinese Academy of Sciences — *Beijing, China*

PhD, Engineering Thermophysics — *Aug 2017–Aug 2023*

- Built coupled experimental–computational workflows for heterogeneous and photo-catalytic systems, spanning DFT, micro-kinetics, and lab-scale reactor design.
- Created bespoke photocatalytic and photolysis reactors that increased quantum efficiency by up to 35% versus legacy rigs.
- Authored 8+ peer-reviewed articles through collaborations with CAS institutes and international partners; dissertation centred on data-driven catalyst discovery for sustainable energy.

University of Engineering and Technology — *Lahore, Pakistan*

BSc, Mechanical Engineering (Fluid Dynamics) — *Aug 2012–Aug 2016*

- Graduated with specialisation in fluid dynamics; capstone coursework in thermodynamics, heat transfer, and energy systems.
- Completed industry-sponsored design projects utilising CAD/CAM, CFD, and experimental validation of thermal processes.

Professional Experience

University Mohammed VI Polytechnic (UM6P) — *Ben Guerir, Morocco*

Postdoctoral Researcher, Chemical and Biochemical Sciences — *2025–Present*

- Steer multi-institutional hydrogen production and CO_2 valorisation programmes from concept to pilot scale, aligning project milestones with national energy-transition initiatives.
- Build automated DFT, molecular dynamics, and micro-kinetic pipelines on UM6P's HPC cluster to interrogate catalyst stability and reaction pathways.
- Deploy machine learning and LLM tools to shortlist catalyst formulations, reducing experimental screening time by ~40%.

Institute of Engineering Thermophysics, Chinese Academy of Sciences — *Beijing, China*

Postdoctoral Researcher — *2023–2024*

- Mentored a cohort of 5+ international researchers, instituting lab protocols that improved catalytic test repeatability by 25%.
- Co-led CO oxidation and methane activation campaigns, delivering three peer-reviewed papers and two invited talks.
- Managed partnerships and instrumentation sharing across CAS institutes, doubling collaborative project inflow.

Pakistan Industrial Technical Assistance Centre (PITAC) — *Lahore, Pakistan*

Intern Engineer — *2016–2017*

- Supported CAD/CAM workflows and produced fabrication drawings for bespoke tooling projects.
- Documented test procedures and liaised with senior engineers to implement design refinements for thermal systems.

Skills

Computational	Density Functional Theory (DFT), Quantum ESPRESSO, VASP, Gaussian; Molecular Dynamics (LAMMPS) Microkinetic Modeling (Cantera, Chemkin); Python; HPC; Git, Bash (Shell), LaTeX
Experimental/Analytical	XRD, XPS, Raman, BET, SEM/EDS; Sol-gel, CVD; CO Oxidation, Photocatalysis
Research Interests	Hydrogen production, CO_2 valorization, Heterogeneous catalysis, Photocatalysis, Machine learning in chemistry
General/Technical	Technical writing, Adobe Illustrator vector drawing, CAD/CAM, Application studies, Research supervision
Languages	English (Fluent), Urdu (Native), Mandarin (Conversational)

Selected Publications

Journal Articles (11 publications)

- Yousuf M, **Arshad MF**, Tian Z-Y. (2024). Thermodynamic properties calculations of Cu-based species. *Int J Chem Kinet.* 56: 310–322.
- El Kasmi A, **Arshad MF**, Waqas M, et al. (2023). Insights into catalytic oxidation mechanism of CO over Cu catalyst. *Materials Research Bulletin*, 112343.
- **Arshad MF**, El Kasmi A, Fonzeu Monguen CK, et al. (2023). Insights into the Role of Carbonates and Hydroxides in La-Co Oxides for CO Catalytic Conversion. *ES Energy & Environment* 20: 908.
- Fonzeu Monguen CK, El Kasmi A, **Arshad MF**, et al. (2022). Oxidative Dehydrogenation of Propane into Propene over Chromium Oxides. *Ind & Eng Chem Research*, 61(13), 4546–4560.
- **Arshad MF**, Wu LN, El Kasmi A, et al. (2021). Ab Initio Calculation of Surface Thermochemistry for Popular Solid Transition Metal-Based Species. *ACS Omega*, 6(35), 22525–22536.
- **Arshad MF**, El Kasmi A, Waqas M, Tian ZY. (2021). Insight into one-step synthesis of active amorphous La-Co thin films for catalytic oxidation of CO. *Applications in Energy and Combustion Science*, 5, 100021.
- Wu LN, Tian ZY, Kasmi A el, **Arshad MF**, Qin W. (2021). Mechanistic study of the CO oxidation reaction on the CuO (111) surface. *Proceedings of the Combustion Institute*, 38(4), 5289–5297.
- Waqas M, El Kasmi A, Wu LN, **Arshad MF**, et al. (2021). Catalytic combustion of CO over Cu-doped iron oxides: CO_2 effects on activity. *Fuel*, 289, 119760.

Full publication list available on Google Scholar and ORCID profiles.

Conferences & Presentations

2021	**European Combustion Meeting**, **Arshad MF**, Wu LN, El Kasmi A, Qin W, Tian ZY. Ab Initio Calculation of Surface Thermochemistry for Popular Solid Transition Metal-Based Species	*Australia*
2020	**Chinese Combustion Symposium**, **Arshad MF**, El Kasmi A, Waqas M, Tian ZY. Insight into one-step synthesis of active amorphous La-Co thin films for catalytic oxidation of CO	*Tianjin, China*

Teaching Experience

University of Chinese Academy of Sciences — *Beijing, China*

Graduate Teaching Assistant, Department — *2020–2021*

- Taught postgraduate students and assisted faculty with course delivery and curriculum development.
- Helped with teaching, examination preparation, and homework grading for advanced courses.
- Provided one-on-one mentoring and guidance to graduate students on research methodologies.
- Facilitated laboratory sessions and supervised experimental work in thermophysics and catalysis.

Awards & Honors

2022	**Outstanding International Student**, UCAS	*Beijing, China*
2020–2024	**CAS–TWAS Fellowship**, The World Academy of Sciences	*Beijing, China*
2017–2020	**Belt and Road Fellowship**, UCAS	*Beijing, China*
2016	**Top Crisis Manager**, University of Engineering and Technology	*Lahore, Pakistan*

Leadership & Services

Institute of Engineering Thermophysics, Chinese Academy of Sciences — *Beijing, China*

Leader of International Staff and Students — *2021–2024*

- Organized weekly meetings to coordinate research activities and foster collaboration among international researchers.
- Provided comprehensive support for research projects, experiments, and computational calculations.
- Facilitated knowledge transfer and skills development within the international research community.
- Served as liaison between international researchers and laboratory management.

University of Chinese Academy of Sciences - International Student Office — *Beijing, China*

Student Guide and Translator — *2017–2023*

- Guided international students and assisted in organizing orientation programs and cultural events.
- Provided translation services from Mandarin to English for academic and administrative purposes.
- Helped international students navigate university systems and integrate into academic life.
- Contributed to improving cross-cultural communication and understanding.

Digital Identifier Links

Research Profiles:

- **ORCID:** 0000-0003-1828-9458
- **Scopus ID:** 57219161795
- **Google Scholar:** fwiNZasAAAAJ
- **Web of Science Researcher ID:** rid102402
- **ResearchGate:** Muhammad-Fahad-Arshad

References: Available upon request. Please contact for details.